On Sum–Connectivity Index of Bicyclic Graphs

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Abstract

We determine the minimum sum–connectivity index of bicyclic graphs with n vertices and matching number m, where $2 \leq m \leq \lfloor \frac{n}{2} \rfloor$, the minimum and the second minimum, as well as the maximum and the second maximum sum–connectivity indices of bicyclic graphs with $n \geq 5$ vertices. The extremal graphs are characterized.

MSC 2000: 05C90; 05C35; 05C07

Keywords: Sum–connectivity index; Randić connectivity index; Matching number; Bicyclic graphs

1 Introduction

The Randić connectivity index [8] is one of the most successful molecular descriptors in structure–property and structure–activity relationships studies, e.g., [9, 10]. Its mathematical properties as well as those of its generalizations have been studied extensively as summarized in the books [6, 5]. Recently, a closely related variant of Randić connectivity index called the sum–connectivity index was proposed in [14].

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Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $d_G(u)$ denotes the degree of u in G. The Randić connectivity index (or product–connectivity index [14, 7]) of the graph G is defined as [8]

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}\,.$$

The sum–connectivity index of G is defined as [14]

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}\,.$$

It has been found that the sum–connectivity index and the Randić connectivity index correlate well among themselves and with π-electronic energy of benzenoid hydrocarbons [14, 7]. Some mathematical properties of the sum–connectivity index have been established in [14, 2, 3]. Recall that an n-vertex connected graph is known as a tree, a unicyclic graph and a bicyclic graph if it possesses $n-1$, n and $n+1$ edges, respectively. In [2], we obtained the minimum sum–connectivity indices of trees and unicyclic graphs respectively with given number of vertices and matching number, and determined the corresponding extremal graphs. The n-vertex trees with the first a few minimum and maximum sum–connectivity indices were determined in [14], while the n-vertex unicyclic graphs with the first a few minimum and maximum sum–connectivity indices were determined in [2] and [3], respectively. In this paper, we consider the sum–connectivity indices of bicyclic graphs.

A matching M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. A matching M of G is said to be maximum, if for any other matching M' of G, $|M'| \leq |M|$. The matching number of G is the number of edges of a maximum matching in G.

If M is a matching of a graph G and vertex $v \in V(G)$ is incident with an edge of M, then v is said to be M-saturated, and if every vertex of G is M-saturated, then M is a perfect matching.

In this paper, we obtain the minimum sum–connectivity index in the set of bicyclic graphs with n vertices and matching number m, where $2 \leq m \leq$

$\lfloor n/2 \rfloor$. We also determine the minimum and the second minimum, as well as the maximum and the second maximum sum–connectivity indices in the set of bicyclic graphs with $n \geq 5$ vertices. The extremal graphs are characterized.

Study on the Randić connectivity indices of bicyclic graphs may be found in [6, 15, 1, 12], and in particular, the minimum and the maximum Randić connectivity indices in the set of bicyclic graphs with $n \geq 5$ vertices were determined in [12] and [1], respectively.

We note that some other graph invariants based on end–vertex degrees of edges in a graph have been studied recently, see, e.g., [4, 11, 13].

2 Preliminaries

For $2 \leq m \leq \lfloor n/2 \rfloor$, let $\mathcal{B}(n, m)$ be the set of bicyclic graphs with n vertices and matching number m.

For $3 \leq m \leq \lfloor n/2 \rfloor$, let $B_{n,m}$ be the graph obtained by identifying a vertex of two triangles, and attaching $n - 2m + 1$ pendent vertices (vertices of degree one) and $m - 3$ paths on two vertices to the common vertex of the two triangles, see Fig. 1. Obviously, $B_{n,m} \in \mathcal{B}(n, m)$.

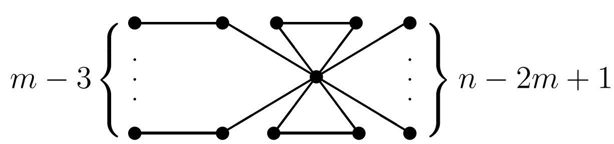

Fig. 1. The graph $B_{n,m}$.

Let C_n ba a cycle on $n \geq 3$ vertices. Let $\widetilde{\mathbb{B}}(n)$ be the set of n-vertex bicyclic graphs without pendent vertices, where $n \geq 4$. Let $\mathbf{B}_1^{(1)}(n)$ be the set of bicyclic graphs obtained by joining two vertex–disjoint cycles C_a and C_b with $a + b = n$ by an edge, where $n \geq 6$. Let $\mathbf{B}_1^{(2)}(n)$ be the set of bicyclic graphs obtained by joining two vertex–disjoint cycles C_a and C_b with $a+b < n$ by a path of length $n - a - b + 1$, where $n \geq 7$. Let $\mathbf{B}_2(n)$ be the set of

bicyclic graphs obtained by identifying a vertex of C_a and a vertex of C_b with $a + b = n + 1$, where $n \geq 5$. Let $\mathbf{B}_3^{(1)}(n)$ be the set of bicyclic graphs obtained from C_n by adding an edge, where $n \geq 4$. Let $\mathbf{B}_3^{(2)}(n)$ be the set of bicyclic graphs obtained by joining two non-adjacent vertices of C_a with $4 \leq a \leq n - 1$ by a path of length $n - a + 1$, where $n \geq 5$. Obviously, $\widetilde{\mathbb{B}}(n) = \mathbf{B}_1^{(1)}(n) \cup \mathbf{B}_1^{(2)}(n) \cup \mathbf{B}_2(n) \cup \mathbf{B}_3^{(1)}(n) \cup \mathbf{B}_3^{(2)}(n)$.

Let $\mathbb{B}(n)$ be the set of bicyclic graphs on $n \geq 4$ vertices.

3 Minimum sum–connectivity index of bicyclic graphs with given matching number

First we give some lemmas that will be used.

For a graph G with $u \in V(G)$, $G - u$ denotes the graph resulting from G by deleting the vertex u (and its incident edges).

Lemma 3.1 *[2] Let G be an n-vertex connected graph with a pendent vertex u, where $n \geq 4$. Let v be the unique neighbor of u, and let w be a neighbor of v different from u.*

(i) If $d_G(v) = 2$ and there is at most one pendent neighbor of w in G, then

$$\chi(G) - \chi(G - u - v) \geq \frac{d_G(w) - 1}{\sqrt{d_G(w) + 2}} - \frac{d_G(w) - 3}{\sqrt{d_G(w) + 1}} - \frac{1}{\sqrt{d_G(w)}} + \frac{1}{\sqrt{3}}$$

with equality if and only if one neighbor of w has degree one, and the other neighbors of w are of degree two.

(ii) If there are at most k pendent neighbors of v in G, then

$$\chi(G) - \chi(G - u) \geq \frac{d_G(v) - k}{\sqrt{d_G(v) + 2}} + \frac{2k - d_G(v)}{\sqrt{d_G(v) + 1}} - \frac{k - 1}{\sqrt{d_G(v)}}$$

with equality if and only if k neighbors of v have degree one, and the other neighbors of v are of degree two.

Lemma 3.2 *[2] (i) The function* $\frac{x-1}{\sqrt{x+2}} - \frac{x-3}{\sqrt{x+1}} - \frac{1}{\sqrt{x}}$ *is decreasing for* $x \geq 2$.

(ii) For integer $a \geq 1$*, the function* $\frac{x-a}{\sqrt{x+2}} + \frac{2a-x}{\sqrt{x+1}} - \frac{a-1}{\sqrt{x}}$ *is decreasing for* $x \geq a+1$.

Lemma 3.3 *[2] Let* G *be a connected graph with* $uv \in E(G)$*, where* $d_G(u)$*,* $d_G(v) \geq 2$*, and* u *and* v *have no common neighbor in* G*. Let* G_1 *be the graph obtained from* G *by deleting the edge* uv*, identifying* u *and* v*, which is denoted by* w*, and attaching a pendent vertex to* w*. Then* $\chi(G) > \chi(G_1)$.

Lemma 3.4 *For* $m \geq 3$, $m + \frac{4}{\sqrt{6}} - \frac{3}{2} > \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1$*, and for* $m \geq 5$, $(\frac{1}{2} + \frac{1}{\sqrt{6}})m - \frac{1}{2} - \frac{2}{\sqrt{6}} + \sqrt{2} > \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1$.

Proof. Let $f(m) = \left(m + \frac{4}{\sqrt{6}} - \frac{3}{2}\right) - \left(\frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1\right)$ for $m \geq 3$, and let $g(m) = \left[\left(\frac{1}{2} + \frac{1}{\sqrt{6}}\right)m - \frac{1}{2} - \frac{2}{\sqrt{6}} + \sqrt{2}\right] - \left(\frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1\right)$ for $m \geq 5$. Note that $f''(m) = g''(m) = -\frac{3}{4}(m+3)^{-5/2} + (\frac{1}{4}m + \frac{13}{4})(m+4)^{-5/2} > 0$. Then $f'(m) \geq f'(3) > 0$, implying that $f(m) \geq f(3) > 0$, and $g'(m) \geq g'(5) > 0$, implying that $g(m) \geq g(5) > 0$. $\square$

Lemma 3.5 *For* $m \geq 3$,

$$-\frac{m+1}{\sqrt{m+4}} + \frac{m-1}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} \geq -\frac{4}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}$$

with equality if and only if $m = 3$.

Proof. Let $f(m) = (m+2)^{-1/2} + m \cdot (m+3)^{-1/2}$ for $m \geq 3$. Then $f''(m) = \frac{3}{4}(m+2)^{-5/2} - (\frac{1}{4}m + 3)(m+3)^{-5/2} < 0$, implying that $f(m) - f(m+1)$ is increasing on m. It is easily seen that

$$\begin{aligned} & -\frac{m+1}{\sqrt{m+4}} + \frac{m-1}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} \\ = \ & f(m) - f(m+1) \\ \geq \ & f(3) - f(4) \\ = \ & -\frac{4}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}} \end{aligned}$$

with equality if and only if $m = 3$. $\square$

Let H_6 be the graph obtained by attaching a pendent vertex to every vertex of a triangle. For $2 \le m \le \lfloor n/2 \rfloor$, let $U_{n,m}$ be the unicyclic graph obtained by attaching $n - 2m + 1$ pendent vertices and $m - 2$ paths on two vertices to one vertex of a triangle.

Lemma 3.6 *[2] Let G be a unicyclic graph with $2m$ vertices and perfect matching, where $m \ge 3$. Suppose that $G \ne H_6$. Then*

$$\chi(G) \ge \frac{m}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} + \frac{m-2}{\sqrt{3}} + \frac{1}{2}$$

with equality if and only if $G = U_{2m,m}$.

For an edge uv of the graph G (the complement of G, respectively), $G-uv$ ($G+uv$, respectively) denotes the graph resulting from G by deleting (adding, respectively) the edge uv.

Lemma 3.7 *Let $G \in \mathcal{B}(2m, m)$ and no pendent vertex has neighbor of degree two, where $m \ge 3$. Then $\chi(G) \ge \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1$ with equality if and only if $m = 3$ and $G = B_{6,3}$.*

Proof. Let $f(m) = \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1$.

Since $G \in \mathcal{B}(2m, m)$ and no pendent vertex has neighbor of degree two, G is obtainable by attaching some pendent vertices to a graph in $\widetilde{\mathbb{B}}(k)$, where $m \le k \le 2m$, and any two pendent vertices have no common neighbor (if $k = 2m$, then no pendent vertex is attached).

Case 1. There is no vertex of degree two in G. Then either $k = m$, G is obtainable by attaching a pendent vertex to every vertex of a graph in $\widetilde{\mathbb{B}}(m)$, or $k = m+1$, G is obtainable by attaching a pendent vertex to every vertex with degree two of a graph in $\mathbf{B}_1^{(1)}(m+1) \cup \mathbf{B}_3^{(1)}(m+1)$. By direct calculation, we find that $\chi(G) = \frac{5}{\sqrt{6}} + 1 > f(3)$ for $m = 3$, $\chi(G) \ge \frac{1}{\sqrt{8}} + \frac{4}{\sqrt{7}} + \frac{2}{\sqrt{5}} + 1 > f(4)$ for $m = 4$, and $\chi(G) \ge \left(\frac{1}{2} + \frac{1}{\sqrt{6}}\right) m - \frac{1}{2} - \frac{2}{\sqrt{6}} + \sqrt{2}$ for $m \ge 5$. Thus by Lemma 3.4, we have $\chi(G) > f(m)$.

Case 2. There is a vertex, say u, of degree two in G. Denote by v and w the two neighbors of u in G. Then one of the two edges incident with u, say $uv \in M$, where M is a perfect matching of G. Suppose that there is no vertex of degree two in any cycle of G. Since no pendent vertex has neighbor of degree two in G, u lies on the path joining the two disjoint cycles of G. For $G_1 = G - uw + vw \in \mathcal{B}(2m, m)$, the difference of the numbers of vertices of degree two outside any cycle of G and G_1 is equal to one, and thus by Lemma 3.3, $\chi(G_1) < \chi(G)$. Repeating the operation from G to G_1, we finally get a graph $G' \in \mathcal{B}(2m, m)$, which has no vertex of degree two, such that $\chi(G) > \chi(G')$, and thus the result follows from Case 1. Now suppose that u lies on some cycle of G. Consider $G' = G - uw$, which is a unicyclic graph with perfect matching. If $G' = H_6$, then G is obtained from H_6 by adding an edge either between two pendent vertices, and thus $\chi(G) = \frac{3}{\sqrt{6}} + \frac{2}{\sqrt{5}} + 1$, or between two neighbors of a vertex of degree three, one of which being a pendent vertex, and thus $\chi(G) = \frac{2}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{1}{2}$. In either case, $\chi(G) > f(3)$. Suppose that $G' \neq H_6$. Then by Lemma 3.6, $\chi(G') \geq \frac{m}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} + \frac{m-2}{\sqrt{3}} + \frac{1}{2}$. Note that $2 \leq d_G(v), d_G(w) \leq 5$ and w has at most one pendent neighbor. By Lemmas 3.2 (i) and 3.5, we have

$$
\begin{aligned}
\chi(G) &= \chi(G') + \frac{1}{\sqrt{d_G(w)+2}} + \left(\frac{1}{\sqrt{d_G(v)+2}} - \frac{1}{\sqrt{d_G(v)+1}}\right) \\
&\quad + \sum_{xw \in E(G')} \left(\frac{1}{\sqrt{d_G(w)+d_G(x)}} - \frac{1}{\sqrt{d_G(w)+d_G(x)-1}}\right) \\
&\geq \chi(G') + \frac{1}{\sqrt{d_G(w)+2}} + \left(\frac{1}{\sqrt{2+2}} - \frac{1}{\sqrt{2+1}}\right) \\
&\quad + \left[\frac{1}{\sqrt{d_G(w)+1}} - \frac{1}{\sqrt{d_G(w)+1-1}}\right. \\
&\quad \left. +(d_G(w)-2)\left(\frac{1}{\sqrt{d_G(w)+2}} - \frac{1}{\sqrt{d_G(w)+2-1}}\right)\right] \\
&= \chi(G') + \left(\frac{d_G(w)-1}{\sqrt{d_G(w)+2}} - \frac{d_G(w)-3}{\sqrt{d_G(w)+1}} - \frac{1}{\sqrt{d_G(w)}}\right) + \frac{1}{2} - \frac{1}{\sqrt{3}}
\end{aligned}
$$

$$
\begin{aligned}
&\ge \left(\frac{m}{\sqrt{m+3}}+\frac{1}{\sqrt{m+2}}+\frac{m-2}{\sqrt{3}}+\frac{1}{2}\right)\\
&\quad+\left(\frac{5-1}{\sqrt{5+2}}-\frac{5-3}{\sqrt{5+1}}-\frac{1}{\sqrt{5}}\right)+\frac{1}{2}-\frac{1}{\sqrt{3}}\\
&= \frac{m}{\sqrt{m+3}}+\frac{1}{\sqrt{m+2}}+\frac{m-2}{\sqrt{3}}+1-\frac{1}{\sqrt{3}}+\left(\frac{4}{\sqrt{7}}-\frac{2}{\sqrt{6}}-\frac{1}{\sqrt{5}}\right)\\
&\ge \frac{m}{\sqrt{m+3}}+\frac{1}{\sqrt{m+2}}+\frac{m-2}{\sqrt{3}}+1-\frac{1}{\sqrt{3}}\\
&\quad+\left(\frac{m+1}{\sqrt{m+4}}-\frac{m-1}{\sqrt{m+3}}-\frac{1}{\sqrt{m+2}}\right)\\
&= f(m)
\end{aligned}
$$

with equalities if and only if $d_G(v)=2$, $d_G(w)=5$, $G'=U_{2m,m}$ and $m=3$, i.e., $G=B_{6,3}$.

By combining Cases 1 and 2, the result follows. □

Lemma 3.8 *Let $G\in\mathcal{B}(6,3)$. Then $\chi(G)\ge\frac{4}{\sqrt{7}}+\frac{1}{\sqrt{6}}+1$ with equality if and only if $G=B_{6,3}$.*

Proof. If G has a pendent vertex whose neighbor is of degree two, then G is the graph obtained from the unique 4-vertex bicyclic graph by attaching a path on two vertices to either a vertex of degree three, or a vertex of degree two, and thus it is easily seen that $\chi(G)>\frac{4}{\sqrt{7}}+\frac{1}{\sqrt{6}}+1$. Otherwise, by Lemma 3.7, $B_{6,3}$ is the unique graph with the minimum sum–connectivity index. □

Now we consider the bicyclic graphs with perfect matching. There is a unique bicyclic graph with four vertices, and its matching number is two.

Theorem 3.1 *Let $G\in\mathcal{B}(2m,m)$, where $m\ge 3$. Then*

$$\chi(G)\ge\frac{m+1}{\sqrt{m+4}}+\frac{1}{\sqrt{m+3}}+\frac{m-3}{\sqrt{3}}+1$$

with equality if and only if $G=B_{2m,m}$.

Proof. Let $f(m) = \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1$. We prove the result by induction on m. If $m = 3$, then the result follows from Lemma 3.8.

Suppose that $m \geq 4$ and the result holds for graphs in $\mathcal{B}(2m-2, m-1)$. Let $G \in \mathcal{B}(2m, m)$ with a perfect matching M.

If there is no pendent vertex with neighbor of degree two in G, then by Lemma 3.7, $\chi(G) > f(m)$. Suppose that G has a pendent vertex u whose neighbor v is of degree two. Then $uv \in M$ and $G-u-v \in \mathcal{B}(2m-2, m-1)$. Let w be the neighbor of v different from u. Since $|M| = m$, we have $d_G(w) \leq m+2$. Note that there is at most one pendent neighbor of w in G. Then by Lemma 3.1 (i), Lemma 3.2 (i) and the induction hypothesis,

$$\begin{aligned} \chi(G) &\geq \chi(G-u-v) + \frac{d_G(w)-1}{\sqrt{d_G(w)+2}} - \frac{d_G(w)-3}{\sqrt{d_G(w)+1}} - \frac{1}{\sqrt{d_G(w)}} + \frac{1}{\sqrt{3}} \\ &\geq f(m-1) + \frac{(m+2)-1}{\sqrt{(m+2)+2}} - \frac{(m+2)-3}{\sqrt{(m+2)+1}} - \frac{1}{\sqrt{m+2}} + \frac{1}{\sqrt{3}} \\ &= f(m) \end{aligned}$$

with equalities if and only if $G-u-v = B_{2m-2,m-1}$ and $d_G(w) = m+2$, i.e., $G = B_{2m,m}$. $\square$

In the following we consider the sum–connectivity indices of graphs in the set of bicyclic graphs with n vertices and matching number m. We first consider the case $m \geq 3$.

Lemma 3.9 *[15] Let $G \in \mathcal{B}(n, m)$ with $n > 2m \geq 6$, and G has at least one pendent vertex. Then there is a maximum matching M and a pendent vertex u such that u is not M-saturated.*

Theorem 3.2 *Let $G \in \mathcal{B}(n, m)$, where $3 \leq m \leq \lfloor n/2 \rfloor$. Then*

$$\chi(G) \geq \frac{m+1}{\sqrt{n-m+4}} + \frac{n-2m+1}{\sqrt{n-m+3}} + \frac{m-3}{\sqrt{3}} + 1$$

with equality if and only if $G = B_{n,m}$.

Proof. Let $f(n,m) = \frac{m+1}{\sqrt{n-m+4}} + \frac{n-2m+1}{\sqrt{n-m+3}} + \frac{m-3}{\sqrt{3}} + 1$. We prove the result by induction on n. If $n = 2m$, then the result follows from Theorem 3.1. Suppose that $n > 2m$ and the result holds for graphs in $\mathcal{B}(n-1,m)$. Let $G \in \mathcal{B}(n,m)$.

Suppose that there is no pendent vertex in G. Then $G \in \widetilde{\mathbb{B}}(n)$ and $n = 2m+1$. It is easily seen that there are exactly three values for $\chi(G)$, and thus we have $\chi(G) \geq \chi(H) = m - 1 + \frac{4}{\sqrt{6}}$ with $H \in \mathbf{B}_2(2m+1)$. Let $g(m) = \left(m - 1 + \frac{4}{\sqrt{6}}\right) - f(2m+1,m) = \left(m - 1 + \frac{4}{\sqrt{6}}\right) - \left(\frac{m+1}{\sqrt{m+5}} + \frac{2}{\sqrt{m+4}} + \frac{m-3}{\sqrt{3}} + 1\right)$ for $m \geq 3$. Then $g''(m) = (\frac{1}{4}m + \frac{17}{4})(m+5)^{-5/2} - \frac{3}{2}(m+4)^{-5/2} > 0$, and thus $g'(m) \geq g'(3) > 0$, implying that $g(m) \geq g(3) > 0$, i.e., $m - 1 + \frac{4}{\sqrt{6}} > f(2m+1,m)$. Then $\chi(G) > f(2m+1,m)$.

Suppose that there is at least one pendent vertex in G. By Lemma 3.9, there is a maximum matching M and a pendent vertex u of G such that u is not M-saturated. Then $G - u \in \mathcal{B}(n-1,m)$. Let v be the unique neighbor of u. Since M is a maximum matching, M contains one edge incident with v. Note that there are $n+1-m$ edges of G outside M. Then $d_G(v) - 1 \leq n+1-m$, i.e., $d_G(v) \leq n-m+2$. Let s be the number of pendent neighbors of v in G. Since at least $s-1$ pendent neighbors of v are not M-saturated, we have $s - 1 \leq n - 2m$, i.e., $s \leq n - 2m + 1$. By Lemma 3.1 (ii) with $k = n - 2m + 1$, Lemma 3.2 (ii) and the induction hypothesis,

$$
\begin{aligned}
\chi(G) &\geq \chi(G-u) + \frac{d_G(v) - (n-2m+1)}{\sqrt{d_G(v)+2}} \\
&\quad + \frac{2(n-2m+1) - d_G(v)}{\sqrt{d_G(v)+1}} - \frac{(n-2m+1)-1}{\sqrt{d_G(v)}} \\
&\geq f(n-1,m) + \frac{(n-m+2)-(n-2m+1)}{\sqrt{(n-m+2)+2}} \\
&\quad + \frac{2(n-2m+1)-(n-m+2)}{\sqrt{(n-m+2)+1}} - \frac{(n-2m+1)-1}{\sqrt{n-m+2}} \\
&= f(n,m)
\end{aligned}
$$

with equalities if and only if $G - u = B_{n-1,m}$, $s = n - 2m + 1$ and $d_G(v) = n - m + 2$, i.e., $G = B_{n,m}$. $\square$

Now we consider the sum–connectivity indices of graphs bicyclic graphs matching number two. Let $B_n(a,b)$ be the graph obtained by attaching $a-3$ and $b-3$ pendent vertices to the two vertices of degree three of the unique 4-vertex bicyclic graph, respectively, where $a \geq b \geq 3$, $a+b=n+2$ and $n \geq 4$.

Lemma 3.10 *Among the graphs in $\mathcal{B}(n,2)$ with $n \geq 6$, $B_n(n-1,3)$ and $B_n(n-2,4)$ are respectively the unique graphs with the minimum and the second minimum sum–connectivity indices, which are equal to $\frac{1}{\sqrt{n+2}} + \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{n+1}} + \frac{2}{\sqrt{5}}$ and $\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}$, respectively.*

Proof. Let $G \in \mathcal{B}(n,2)$. Then G may be of three types:

(a) $G = B_n(a,b)$ with $a \geq b \geq 3$. Suppose that $a \geq b \geq 4$. Let $f(x) = (x-4)x^{-1/2} + 2(x+1)^{-1/2}$ for $x \geq 3$. Then $f''(x) = -(\frac{1}{4}x+3)x^{-5/2} + \frac{3}{2}(x+1)^{-5/2} < 0$, implying that $f(x+1)-f(x)$ is decreasing for $x \geq 3$. It is easily seen that

$$\begin{aligned}
& \chi(B_n(a+1,b-1)) - \chi(B_n(a,b)) \\
= \; & [\chi(B_n(a+1,b-1)) - \chi(B_{n-1}(a,b-1))] \\
& -[\chi(B_n(a,b)) - \chi(B_{n-1}(a,b-1))] \\
= \; & \left(\frac{a-4}{\sqrt{a+2}} - \frac{a-3}{\sqrt{a+1}} + \frac{2}{\sqrt{a+3}}\right) - \left(\frac{b-5}{\sqrt{b+1}} - \frac{b-4}{\sqrt{b}} + \frac{2}{\sqrt{b+2}}\right) \\
= \; & [f(a+2) - f(a+1)] - [f(b+1) - f(b)] < 0,
\end{aligned}$$

and thus, $\chi(B_n(a,b)) > \chi(B_n(a+1,b-1))$ for $a \geq b \geq 4$. It follows that $B_n(n-1,3)$ and $B_n(n-2,4)$ are respectively the unique graphs with the minimum and the second minimum sum–connectivity indices, which are equal to $\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n+1}} + \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{5}}$ and $\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}$, respectively.

(b) G is the graph obtained by attaching $n-4$ pendent vertices to a vertex of degree two of the unique 4-vertex bicyclic graph. Then

$$\begin{aligned}
& \chi(G) = \frac{2}{\sqrt{n+1}} + \frac{n-4}{\sqrt{n-1}} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{5}} \\
> \; & \chi(B_n(n-2,4)) = \frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}},
\end{aligned}$$

since $\chi(G) - \chi(B_n(n-2,4)) = [g(n-1) - g(n)] + \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{6}} > 0$, where $g(x) = \frac{1}{\sqrt{x+2}} + \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+1}}$ is decreasing for $x \geq 5$.

(c) G is the graph obtained by attaching some pendent vertices to one or two vertices of degree three of the unique 5-vertex bicyclic graph in $\mathbf{B}_3^{(2)}(5)$, and by Lemma 3.3 and the arguments in case (a), $\chi(G) > \chi(B_n(n-2,4))$.

Now the result follows easily. $\square$

4 Minimum sum–connectivity index of bicyclic graphs

In this section, we determine the minimum and the second minimum sum–connectivity indices of bicyclic graphs with $n \geq 5$ vertices.

Theorem 4.1 *Among the graphs in $\mathbb{B}(n)$ with $n \geq 5$, $B_n(n-1,3)$ is the unique graph with the minimum sum–connectivity index, which is equal to $\frac{1}{\sqrt{n+2}} + \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{n+1}} + \frac{2}{\sqrt{5}}$, the graph obtained by attaching a pendent vertex to a vertex of degree two of the unique 4-vertex bicyclic graph for $n = 5$ is the unique graph with the second minimum sum–connectivity index, which is equal to $\frac{3}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{1}{2}$, $B_n(n-2,4)$ for $n = 6, 7$ is the unique graph with the second minimum sum–connectivity index, which is equal to $\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}$, and $B_{n,3}$ for $n \geq 8$ is the unique graph with the second minimum sum–connectivity index, which is equal to $\frac{4}{\sqrt{n+1}} + \frac{n-5}{\sqrt{n}} + 1$.*

Proof. There are five graphs in $\mathbb{B}(5)$. Thus, the case $n = 5$ may be checked directly. Suppose in the following that $n \geq 6$.

Let $G \in \mathbb{B}(n)$ and m the matching number of G, where $2 \leq m \leq \lfloor n/2 \rfloor$. If $m = 2$, then by Lemma 3.10, $\chi(G) \geq \chi(B_n(n-1,3))$ with equality if and only if $G = B_n(n-1,3)$. If $m = 3$, then by Theorem 3.2, $\chi(G) \geq \chi(B_{n,3})$ with equality if and only if $G = B_{n,3}$. If $m \geq 4$, then by Theorem 3.2 and Lemma 3.3, $\chi(G) \geq \chi(B_{n,m}) > \chi(B_{n,m-1}) > \cdots > \chi(B_{n,3})$. Let $f(x) = \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+1}}$ for $x \geq 6$. Then $f''(x) = \frac{3}{4}x^{-5/2} - \frac{3}{4}(x+1)^{-5/2} > 0$, implying that $f(x+1) - f(x)$

is increasing for $x \geq 6$. Note that

$$\begin{aligned}
& \chi(B_{n,3}) - \chi(B_n(n-1,3)) \\
= \; & \left(\frac{4}{\sqrt{n+1}} + \frac{n-5}{\sqrt{n}} + 1\right) - \left(\frac{1}{\sqrt{n+2}} + \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{n+1}} + \frac{2}{\sqrt{5}}\right) \\
= \; & f(n+1) - f(n) + 1 - \frac{2}{\sqrt{5}} \\
\geq \; & f(7) - f(6) + 1 - \frac{2}{\sqrt{5}} > 0.
\end{aligned}$$

Thus $B_n(n-1,3)$ is the unique graph with the minimum sum–connectivity index.

Suppose that $G \neq B_n(n-1,3)$. If $m = 2$, then by Lemma 3.10, $\chi(G) \geq \chi(B_n(n-2,4))$ with equality if and only if $G = B_n(n-2,4)$. By the arguments as above, the second minimum sum–connectivity index of graphs in $\mathbb{B}(n)$ is precisely achieved by the minimum one of $\chi(B_{n,3})$ and $\chi(B_n(n-2,4))$. If $n = 6, 7$, then $\chi(B_{n,3}) > \chi(B_n(n-2,4))$. Suppose that $n \geq 8$. Let $g(x) = \frac{1}{\sqrt{x+1}} - \frac{3}{\sqrt{x}} - \frac{x-5}{\sqrt{x-1}}$ for $x \geq 8$. Then $g''(x) = \frac{3}{4}(x+1)^{-5/2} + \left[(\frac{1}{4}x + \frac{11}{4})(x-1)^{-5/2} - \frac{9}{4}x^{-5/2}\right] > 0$, implying that $g(x) - g(x+1)$ is decreasing for $x \geq 8$. Note that

$$\begin{aligned}
& \chi(B_{n,3}) - \chi(B_n(n-2,4)) \\
= \; & \left(\frac{4}{\sqrt{n+1}} + \frac{n-5}{\sqrt{n}} + 1\right) - \left(\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}\right) \\
= \; & -\frac{1}{\sqrt{n+2}} + \frac{4}{\sqrt{n+1}} + \frac{n-7}{\sqrt{n}} - \frac{n-5}{\sqrt{n-1}} + 1 - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{5}} \\
= \; & g(n) - g(n+1) + 1 - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{5}} \\
\leq \; & g(8) - g(9) + 1 - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{5}} < 0,
\end{aligned}$$

and then $\chi(B_{n,3}) < \chi(B_n(n-2,4))$. Thus $B_n(n-2,4)$ for $n = 6, 7$ and $B_{n,3}$ for $n \geq 8$ are the unique graphs with the second minimum sum–connectivity index among graphs in $\mathbb{B}(n)$. $\square$

5 Maximum sum–connectivity index of bicyclic graphs

In this section, we determine the maximum and the second maximum sum–connectivity indices of bicyclic graphs with $n \geq 5$ vertices. Let P_n be the path on n vertices.

Lemma 5.1 *[14] For a connected graph Q with at least two vertices and a vertex $u \in V(Q)$, let G_1 be the graph obtained from Q by attaching two paths P_a and P_b to u, G_2 the graph obtained from Q by attaching a path P_{a+b} to u, where $a \geq b \geq 1$. Then $\chi(G_1) < \chi(G_2)$.*

Lemma 5.2 *Suppose that M is a connected graph with $u \in V(M)$ and $2 \leq d_M(u) \leq 4$. Let H be the graph obtained from M by attaching a path P_a to u. Denote by u_1 and u_2 the two neighbors of u in M, and u' the pendent vertex of the path attached to u in H. Let $H' = H - uu_2 + u'u_2$.*

(i) If $d_M(u) = 2$ and the maximum degree of M is at most five, then $\chi(H') > \chi(H)$.

(ii) If $d_M(u) = 3$, and there are at least two neighbors of u in M with degree two and $d_M(u_2) = 2$, then $\chi(H') > \chi(H)$.

(iii) If $d_M(u) = 4$ and all the neighbors of u in M are of degree two, then $\chi(H') > \chi(H)$.

Proof. (i) If $a = 1$, then

$$\begin{aligned} & \chi(H') - \chi(H) \\ = & \left(\frac{1}{\sqrt{d_M(u_1)+2}} + \frac{1}{\sqrt{d_M(u_2)+2}}\right) - \left(\frac{1}{\sqrt{d_M(u_1)+3}} + \frac{1}{\sqrt{d_M(u_2)+3}}\right) \\ > & \ 0. \end{aligned}$$

If $a \geq 2$, then

$$\chi(H') - \chi(H)$$

$$
\begin{aligned}
&= \left(\frac{1}{\sqrt{d_M(u_1)+2}} - \frac{1}{\sqrt{d_M(u_1)+3}}\right) + \left(\frac{1}{\sqrt{d_M(u_2)+2}} - \frac{1}{\sqrt{d_M(u_2)+3}}\right) \\
&\quad +1 - \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{5}} \\
&\geq \left(\frac{1}{\sqrt{5+2}} - \frac{1}{\sqrt{5+3}}\right) + \left(\frac{1}{\sqrt{5+2}} - \frac{1}{\sqrt{5+3}}\right) + 1 - \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{5}} > 0.
\end{aligned}
$$

(ii) There are two neighbors of u with degree two, let d_1 be the degree of the third neighbor of u in M. If $a = 1$, then since $\frac{1}{2} + \frac{1}{\sqrt{5}} - \frac{2}{\sqrt{6}} > 0$, we have

$$
\begin{aligned}
&\chi(H') - \chi(H) \\
&= \left(\frac{1}{\sqrt{d_1+3}} + \frac{1}{2} + \frac{2}{\sqrt{5}}\right) - \left(\frac{1}{\sqrt{d_1+4}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}\right) \\
&= \left(\frac{1}{\sqrt{d_1+3}} - \frac{1}{\sqrt{d_1+4}}\right) + \frac{1}{2} + \frac{1}{\sqrt{5}} - \frac{2}{\sqrt{6}} > 0.
\end{aligned}
$$

If $a \geq 2$, then since $1 + \frac{2}{\sqrt{5}} - \frac{3}{\sqrt{6}} - \frac{1}{\sqrt{3}} > 0$, we have

$$
\begin{aligned}
&\chi(H') - \chi(H) \\
&= \left(\frac{1}{\sqrt{d_1+3}} + 1 + \frac{2}{\sqrt{5}}\right) - \left(\frac{1}{\sqrt{d_1+4}} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}}\right) \\
&= \left(\frac{1}{\sqrt{d_1+3}} - \frac{1}{\sqrt{d_1+4}}\right) + 1 + \frac{2}{\sqrt{5}} - \frac{3}{\sqrt{6}} - \frac{1}{\sqrt{3}} > 0.
\end{aligned}
$$

(iii) If $a = 1$, then

$$\chi(H') - \chi(H) = \left(\frac{1}{2} + \frac{4}{\sqrt{6}}\right) - \left(\frac{4}{\sqrt{7}} + \frac{1}{\sqrt{6}}\right) > 0.$$

If $a \geq 2$, then

$$\chi(H') - \chi(H) = \left(1 + \frac{4}{\sqrt{6}}\right) - \left(\frac{5}{\sqrt{7}} + \frac{1}{\sqrt{3}}\right) > 0.$$

The proof is now completed. $\square$

Let $\mathbb{B}_1(n)$ be the set of connected graphs on $n \geq 6$ vertices with exactly two vertex–disjoint cycles. Let $\mathbb{B}_2(n)$ be the set of connected graphs on $n \geq 5$

vertices with exactly two cycles of a common vertex. Let $\mathbb{B}_3(n)$ be the set of connected graphs on $n \geq 4$ vertices with exactly two cycles with at least one edge in common. Obviously, $\mathbb{B}(n) = \mathbb{B}_1(n) \cup \mathbb{B}_2(n) \cup \mathbb{B}_3(n)$. For $u, v \in V(G)$, let $d_G(u, v)$ be the distance between u and v in G.

Lemma 5.3 *Among the graphs in $\mathbb{B}_1(n)$ with $n \geq 7$, the graphs in $\mathbf{B}_1^{(1)}(n)$ and the graphs in $\mathbf{B}_1^{(2)}(n)$ are respectively the unique graphs with the maximum and the second maximum sum–connectivity indices, which are equal to $\frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}}$ and $\frac{n-5}{2} + \frac{6}{\sqrt{5}}$, respectively.*

Proof. Suppose that G is a graph in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with the maximum sum–connectivity index, and $C^{(1)}$ and $C^{(2)}$ are its two cycles. Let $x_1 \in V\left(C^{(1)}\right)$ and $y_1 \in V\left(C^{(2)}\right)$ be the two vertices such that $d_G(x_1, y_1) = \min\{d_G(x, y) : x \in V\left(C^{(1)}\right), y \in V\left(C^{(2)}\right)\}$. Let Q be the path joining x_1 and y_1. By Lemma 5.1, the vertices outside $C^{(1)}$, $C^{(2)}$ and Q are of degree one or two, the vertices on $C^{(1)}$, $C^{(2)}$ and Q different from x_1 and y_1 are of degree two or three, and $d_G(x_1), d_G(y_1) = 3$ or 4.

Suppose that $d_G(x_1, y_1) \geq 2$. If there is some vertex, say x, on $C^{(1)}$, $C^{(2)}$ or Q different from x_1 and y_1 with degree three, then making use of Lemma 5.2 (i) to $H = G$ by setting $u = x$, we may get a graph in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with larger sum–connectivity index, a contradiction. Thus the vertices on $C^{(1)}$, $C^{(2)}$ and Q different from x_1 and y_1 are of degree two. If $d_G(x_1) = 4$, then making use of Lemma 5.2 (ii) to $H = G$ by setting $u = x_1$, we may get a graph in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with larger sum–connectivity index, a contradiction. Thus $d_G(x_1) = 3$. Similarly, we have $d_G(y_1) = 3$. It follows that $G \in \mathbf{B}_1^{(2)}(n)$.

Suppose that $d_G(x_1, y_1) = 1$. Suppose that one of x_1 and y_1, say x_1, is of degree four. Then by Lemma 5.2 (i), the vertices on $C^{(1)}$ and $C^{(2)}$ different from x_1 and y_1 are of degree two. If $d_G(y_1) = 4$, then making use of Lemma 5.2 (ii) to $H = G$ by setting $u = y_1$, we may get a graph in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with larger sum–connectivity index, a contradiction. Thus $d_G(y_1) = 3$. Denote by x_2 the pendent vertex of the path attached to x_1.

Consider $G_1 = G - x_1y_1 + x_2y_1 \in \mathbf{B}_1^{(2)}(n)$. If $d_G(x_1, x_2) = 1$, then

$$\chi(G_1) - \chi(G) = \frac{4}{\sqrt{5}} - \left(\frac{1}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}\right) > 0.$$

If $d_G(x_1, x_2) \geq 2$, then

$$\chi(G_1) - \chi(G) = \left(\frac{1}{2} + \frac{4}{\sqrt{5}}\right) - \left(\frac{1}{\sqrt{7}} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}}\right) > 0.$$

In either case, $\chi(G_1) > \chi(G)$ with $G_1 \in \mathbf{B}_1^{(2)}(n)$, a contradiction. Thus $d_G(x_1) = d_G(y_1) = 3$. Note that $G \notin \mathbf{B}_1^{(1)}(n)$ and by Lemma 5.2 (i), there is exactly one vertex, say $x_3 \in V\left(C^{(1)}\right)$, on $C^{(1)}$ and $C^{(2)}$ different from x_1 and y_1 with degree three. Denote by x_4 the pendent vertex of the path attached to x_3. Consider $G_2 = G - x_1y_1 + x_4y_1 \in \mathbf{B}_1^{(2)}(n)$. Let d_1 be the degree of the neighbor of x_4, one neighbor of x_1 on $C^{(1)}$ is of degree two, and we denote by d_2 the other degree of the neighbor of x_1 on $C^{(1)}$, where $d_1, d_2 = 2$ or 3. We have

$$\begin{aligned}
& \chi(G_2) - \chi(G) \\
= \ & \left(\frac{1}{\sqrt{d_1+2}} - \frac{1}{\sqrt{d_1+1}}\right) + \left(\frac{1}{\sqrt{d_2+2}} - \frac{1}{\sqrt{d_2+3}}\right) + \frac{1}{2} - \frac{1}{\sqrt{6}} \\
\geq \ & \left(\frac{1}{\sqrt{2+2}} - \frac{1}{\sqrt{2+1}}\right) + \left(\frac{1}{\sqrt{3+2}} - \frac{1}{\sqrt{3+3}}\right) + \frac{1}{2} - \frac{1}{\sqrt{6}} > 0,
\end{aligned}$$

and thus, $\chi(G_2) > \chi(G)$ with $G_2 \in \mathbf{B}_1^{(2)}(n)$, which is also a contradiction.

Now we have shown that the graphs in $\mathbf{B}_1^{(2)}(n)$ are the unique graphs in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with the maximum sum–connectivity index. Note that for $H_1 \in \mathbf{B}_1^{(1)}(n)$ and $H_2 \in \mathbf{B}_1^{(2)}(n)$,

$$\chi(H_1) = \frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}} > \chi(H_2) = \frac{n-5}{2} + \frac{6}{\sqrt{5}}.$$

The result follows. $\square$

Lemma 5.4 *Among the graphs in $\mathbb{B}_3(n)$ with $n \geq 5$, the graphs in $\mathbf{B}_3^{(1)}(n)$ and the graphs in $\mathbf{B}_3^{(2)}(n)$ are respectively the unique graphs with the maximum and the second maximum sum–connectivity indices, which are equal to $\frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}}$ and $\frac{n-5}{2} + \frac{6}{\sqrt{5}}$, respectively.*

Proof. Suppose that G is a graph in $\mathbb{B}_3(n) \setminus \left\{\mathbf{B}_3^{(1)}(n)\right\}$ with the maximum sum–connectivity index. Then G has exactly three cycles, let $C^{(1)}$ and $C^{(2)}$ be its two cycles such that the remaining one is of the maximum length. Let A be the set of the common vertices of $C^{(1)}$ and $C^{(2)}$. Let v_1 and v_2 be the two vertices in A such that $d_G(v_1, v_2) = \max\{d_G(x, y) : x, y \in A\}$. By Lemma 5.1, the vertices outside $C^{(1)}$ and $C^{(2)}$ are of degree one or two, the vertices on $C^{(1)}$ and $C^{(2)}$ different from v_1 and v_2 are of degree two or three, and $d_G(v_1), d_G(v_2) = 3$ or 4. Denote by v_1' (v_2', respectively) the neighbor of v_1 on $C^{(1)}$ (v_2 on $C^{(2)}$, respectively) different from the vertices in A.

If $d_G(v_1, v_2) \geq 2$, then by Lemma 5.2 (i) and (ii), we have $G \in \mathbf{B}_3^{(2)}(n)$.

Suppose that $d_G(v_1, v_2) = 1$. Suppose that the lengths of $C^{(1)}$ and $C^{(2)}$ are at least four. Consider $G_1 = G - \{v_1v_1', v_2v_2'\} + \{v_1'v_2, v_1v_2'\} \in \mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$. Note that

$$\begin{aligned}\chi(G_1) - \chi(G) &= \left(\frac{1}{\sqrt{d_G(v_1') + d_G(v_2)}} + \frac{1}{\sqrt{d_G(v_1) + d_G(v_2')}}\right) \\ &\quad - \left(\frac{1}{\sqrt{d_G(v_1) + d_G(v_1')}} + \frac{1}{\sqrt{d_G(v_2) + d_G(v_2')}}\right).\end{aligned}$$

If $d_G(v_1) = d_G(v_2)$, then $\chi(G_1) = \chi(G)$. If $d_G(v_1) \neq d_G(v_2)$, then by Lemma 5.2 (i), we have $d_G(v_1') = d_G(v_2') = 2$, and thus $\chi(G_1) = \chi(G)$. In either case, we have $\chi(G_1) = \chi(G)$. By Lemma 5.3, we have $\chi(G) = \chi(G_1) \leq \chi(H) = \frac{n-5}{2} + \frac{6}{\sqrt{5}}$ for $H \in \mathbf{B}_1^{(2)}(n)$ with equality if and only if $G_1 \in \mathbf{B}_1^{(2)}(n)$, i.e., $G \in \mathbf{B}_3^{(2)}(n)$.

Suppose that at least one of $C^{(1)}$ and $C^{(2)}$, say $C^{(1)}$, is of length three. Since $G \notin \mathbf{B}_3^{(1)}(n)$, there are some vertices outside $C^{(1)}$ and $C^{(2)}$. By Lemma 5.2 (i) and (ii), the subgraph induced by the vertices outside $C^{(1)}$ and $C^{(2)}$

is a path, say P_k, which is attached to $x \in V\left(C^{(1)}\right) \cup V\left(C^{(2)}\right)$. Suppose that $x \neq v_1'$. Denote by v_3 the neighbor of x outside $C^{(1)}$ and $C^{(2)}$. Consider $G_2 = G - xv_3 + v_1'v_3 \in \mathbb{B}_3(n) \setminus \left\{\mathbf{B}_3^{(1)}(n)\right\}$. If $x = v_1$ or v_2, then

$$\begin{aligned}
&\chi(G_2) - \chi(G) \\
= &\left(\frac{1}{\sqrt{d_G(v_3)+3}} - \frac{1}{\sqrt{d_G(v_3)+4}}\right) + \left(\frac{1}{\sqrt{6}} - \frac{1}{\sqrt{7}}\right) > 0,
\end{aligned}$$

and thus $\chi(G_2) > \chi(G)$, a contradiction. Hence $x \in V\left(C^{(2)}\right) \setminus \{v_1, v_2\}$, and the length of $C^{(2)}$ is at least four. Note that one neighbor of x on $C^{(2)}$ is of degree two. Denote by d_1 the degree of the other neighbor of x on $C^{(2)}$, where $d_1 = 2$ or 3. Then

$$\begin{aligned}
&\chi(G_2) - \chi(G) \\
= &\left(\frac{1}{\sqrt{d_1+2}} - \frac{1}{\sqrt{d_1+3}}\right) + \frac{1}{2} + \frac{2}{\sqrt{6}} - \frac{3}{\sqrt{5}} \\
\geq &\left(\frac{1}{\sqrt{3+2}} - \frac{1}{\sqrt{3+3}}\right) + \frac{1}{2} + \frac{2}{\sqrt{6}} - \frac{3}{\sqrt{5}} > 0,
\end{aligned}$$

and thus $\chi(G_2) > \chi(G)$, which is also a contradiction. Thus, $x = v_1'$. If $k = 1$, then $\chi(G) = \frac{n-5}{2} + \frac{3}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{1}{2}$, and if $k \geq 2$, then $\chi(G) = \frac{n-6}{2} + \frac{3}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \frac{1}{\sqrt{3}}$. In either case, we have $\chi(G) < \frac{n-5}{2} + \frac{6}{\sqrt{5}}$.

Now we have shown that the graphs in $\mathbf{B}_3^{(2)}(n)$ are the unique graphs in $\mathbb{B}_3(n) \setminus \left\{\mathbf{B}_3^{(1)}(n)\right\}$ with the maximum sum–connectivity index. Note that for $H_1 \in \mathbf{B}_3^{(1)}(n)$ and $H_2 \in \mathbf{B}_3^{(2)}(n)$,

$$\chi(H_1) = \frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}} > \chi(H_2) = \frac{n-5}{2} + \frac{6}{\sqrt{5}}.$$

The result follows. $\square$

Theorem 5.1 *Among the graphs in $\mathbb{B}(n)$ with $n \geq 5$, the graph in $\mathbf{B}_3^{(1)}(5)$ and the graph in $\mathbf{B}_3^{(2)}(5)$ for $n = 5$ are respectively the unique graphs with the maximum and the second maximum sum–connectivity indices, the graphs*

in $\mathbf{B}_1^{(1)}(6) \cup \mathbf{B}_3^{(1)}(6)$ *and the graph in* $\mathbf{B}_3^{(2)}(6)$ *for* $n = 6$ *are respectively the unique graphs with the maximum and the second maximum sum–connectivity indices, the graphs in* $\mathbf{B}_1^{(1)}(n) \cup \mathbf{B}_3^{(1)}(n)$ *and the graphs in* $\mathbf{B}_1^{(2)}(n) \cup \mathbf{B}_3^{(2)}(n)$ *for* $n \geq 7$ *are respectively the unique graphs with the maximum and the second maximum sum–connectivity indices, where* $\chi(G) = \frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}}$ *for* $G \in \mathbf{B}_1^{(1)}(n) \cup \mathbf{B}_3^{(1)}(n)$ *and* $\chi(H) = \frac{n-5}{2} + \frac{6}{\sqrt{5}}$ *for* $H \in \mathbf{B}_1^{(2)}(n) \cup \mathbf{B}_3^{(2)}(n)$.

Proof. Suppose that G is a graph in $\mathbb{B}_2(n)$ with the maximum sum–connectivity index, and $C^{(1)}$ and $C^{(2)}$ are its two cycles. Let u be the unique common vertex of $C^{(1)}$ and $C^{(2)}$. By Lemma 5.1, the vertices outside $C^{(1)}$ and $C^{(2)}$ are of degree one or two, the vertices on $C^{(1)}$ and $C^{(2)}$ different from u are of degree two or three, and $d_G(u) = 4$ or 5. Moreover, by Lemma 5.2 (i), the vertices on $C^{(1)}$ and $C^{(2)}$ different from u are of degree two. If $d_G(u) = 5$, then making use of Lemma 5.2 (iii) to $H = G$, we may get a graph in $\mathbb{B}_2(n)$ with larger sum–connectivity index, a contradiction. Thus $d_G(u) = 4$, i.e., $G \in \mathbf{B}_2(n)$.

Note that for $H_1 \in \mathbf{B}_1^{(1)}(n)$, $H_1' \in \mathbf{B}_1^{(2)}(n)$, $H_2 \in \mathbf{B}_2(n)$, $H_3 \in \mathbf{B}_3^{(1)}(n)$ and $H_3' \in \mathbf{B}_3^{(2)}(n)$,

$$\begin{aligned}
& \chi(H_1) = \chi(H_3) = \frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}} \\
> \ & \chi(H_1') = \chi(H_3') = \frac{n-5}{2} + \frac{6}{\sqrt{5}} \\
> \ & \chi(H_2) = \frac{n-3}{2} + \frac{4}{\sqrt{6}}.
\end{aligned}$$

Then the result follows from Lemmas 5.3 and 5.4. □

Acknowledgement. This work was supported by the National Natural Science Foundation of China (Grant No. 10671076).

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